

REPORT DOCUMENTATION PAGE

Public reporting burden for this collection of information is estimated to average 1 hour per response, including gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Service, Paperwork Project, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Project, Suite 1204, Arlington, VA 22202-4302.

AFRL-SR-BL-TR-01-

0174

Source, of this report, AFRL/AFOSR/ASR/20503.

1. AGENCY USE ONLY (Leave blank)		2. REPORT DATE		3. REP		PERIOD COVERED 15 August 1996-31 August 2000	
4. TITLE AND SUBTITLE High-Order Time-Domain Methods for Maxwell's Equations						5. FUNDING NUMBERS F49620-96-1-0426	
6. AUTHOR(S) David Gottlieb							
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Division of Applied Mathematics Brown University 182 George Street Providence, RI 02912						8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) AFOSR 801 N. Randolph Street, Room 732 Arlington, VA 22203-1977						10. SPONSORING/MONITORING AGENCY REPORT NUMBER F49620-96-1-0426	
11. SUPPLEMENTARY NOTES						AIR FORCE OFFICE OF SCIENTIFIC RESEARCH (AFOSR) NOTICE OF TRANSMITTAL DTIC. THIS TECHNICAL REPORT HAS BEEN REVIEWED AND IS APPROVED FOR PUBLIC RELEASE LAW AFR 190-12. DISTRIBUTION IS UNLIMITED.	
12a. DISTRIBUTION AVAILABILITY STATEMENT Approved for Public Release.						12b. DISTRIBUTION CODE	
13. ABSTRACT (Maximum 200 words) A concentrated effort has recently been initiated to develop methods for solving the time domain Maxwell's equations in complex geometries and media using an fully unstructured grid. The USEMe code (Unstructured Spectral Element Method) is the resulting implementation of a numerical scheme which employs nodal high-order/spectral multi-domain methods. Each component of the code has been carefully designed with efficiency, accuracy, flexibility, and robustness in mind. The standard geometric building block by which the computational domain is gridded in USEME is the triangular element in 2D, and the tetrahedral element in 3D. This allows for the use of standard finite element or finite volume type meshes using these elements to describe arbitrarily complex domains, hence overcoming one of the main concerns associated with the structured grid methods. The use of triangles and tetrahedrons remains of the most important design principles of the method as it enables a tight integration with industry standard mesh generators. USEMe is based on penalty/discontinuous Galerkin (DGM) type scheme, which is a particular form of a penalty scheme that guarantees elemental conservation and global stability. Neighboring elements are patched together through the use of penalty terms to account for jumps across their shared boundary. This formulation has the advantage that it allows material coefficients to vary discontinuously at the interface between two elements, while still preserving high order accuracy. Additionally this allows for efficient communication in parallel computations.							
14. SUBJECT TERMS						15. NUMBER OF PAGES 15	
						16. PRICE CODE	
17. SECURITY CLASSIFICATION OF REPORT		18. SECURITY CLASSIFICATION OF THIS PAGE		19. SECURITY CLASSIFICATION OF ABSTRACT		20. LIMITATION OF ABSTRACT	

Final Report for AFOSR/DARPA Grant F49620-96-1-0426

High-Order Time-Domain Methods for Maxwells Equations

Principal Investigator

David Gottlieb
Division of Applied Mathematics
Brown University, Box F
Providence, RI 02912

20010326 128

I. Motivation and Overall Goals

The current interest in the modeling and design of emerging technologies such as very low observable vehicles, ground/foilage penetrating radars and phase sensitive components, imposes requirements on the accuracy and performance of the computational tools far beyond the capabilities of existing techniques. Furthermore, the need to accurately model the interaction of very broad band signals with electrically large and geometrically complex objects, often including regions of advanced materials, suggests that new approaches beyond integral equation based approaches to electromagnetic modeling and design be sought.

As has been realized over the last few years, the widely used finite-difference time-domain (FD-TD) method for the time-domain solution of Maxwells equations has a number of very unfortunate properties. On one hand, the theoretical second order spatial and temporal accuracy requires the use of a significant number of grid points per characteristic wave length to accurately resolve the wave propagation and reflection and refraction at interfaces. This again translates into a very large number of degrees of freedom and makes the modeling of large scale scattering and penetration problems prohibitive. Furthermore, the straightforward use of a simple Cartesian grid structure implies that material interfaces and metallic boundaries be forced to align with the underlying grid structure, hence prohibiting the accurate representation of curved interfaces/boundaries and reducing the accuracy of the scheme to first order. A final, and often overlooked, problem is the inability of the FD-TD approach to enforce the correct jump conditions of the electric and magnetic field components across material interfaces. As can be shown through simple analysis, this reduces the accuracy of the scheme to less than first order and may even result in nonconvergent behavior.

It is to resolve these critical, and crippling, issues that we during the last year have initiated the development of a new generation of high-order/spectral schemes for the time-domain solution of Maxwells equations employing a truly unstructured grid volume representation.

It is well known that the key technique to overcome the numerical errors associated the classical FT-TD approach is to use high-order/spectral accuracy methods, which allows for a dramatic reduction of the number of grid points per characteristic wavelength without sacrificing the overall accuracy, i.e., for a high-order scheme one can typically accurately model the wave phenomena with 4-6 points per wavelength. Geometric flexibility, hence overcoming the problems with representing curvilinear bodies and interfaces, is ensured by using a fully unstructured body-conforming grid which also allows for enforcing the physically correct jump conditions on the individual field components across material interfaces and at metallic boundaries.

The unstructured grid scheme is entirely local and information is only exchanged between faces of elements, i.e., the formulation allows for very efficient parallel implementations, essential to enable the modeling of large complex objects. Furthermore, the use of an standard unstructured grid allows for the tight integration with existing key elements of a design and analysis loop such as grid generation technology, CAD systems and pre- and post-processing analysis tools. This latter point is often underestimated but plays a key role if a transition to a larger user base is to be successful and has therefore been a guiding light throughout the development, initial implementation and verification.

II. Current State of Development and Main Achievements

In the following we shall review the main accomplishments during the period of the project as related to the continued development of high-order/spectral time-domain methods. We shall overview the status of the development of structured grid spectral methods, the more recent

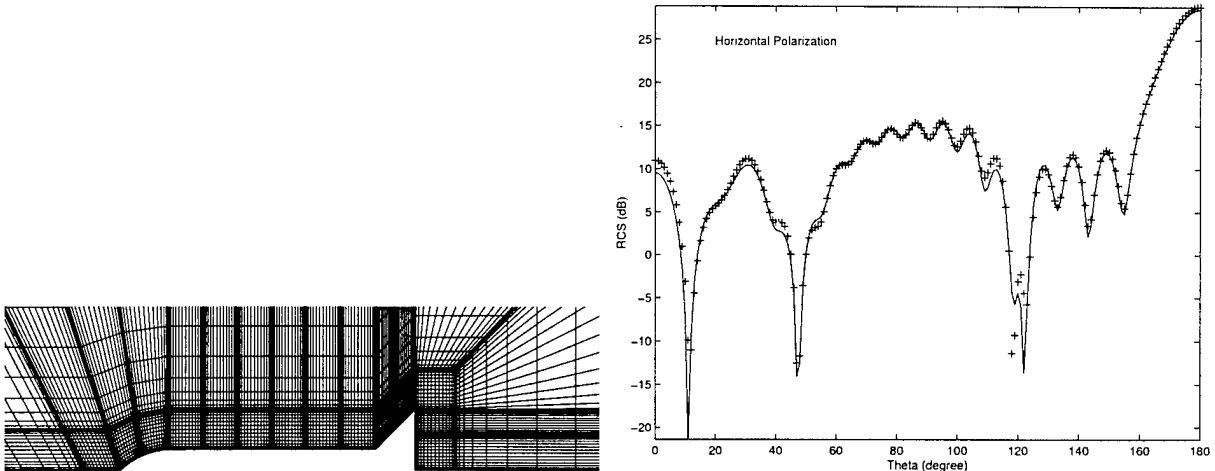


Figure 1: Left: Typical multi-domain grid for the solution of the scattering by a missile. Right: $RCS(\theta,0)$ for a missile subject to axial illumination by a horizontally polarized plane wave. The reference solution, marked by “+”, was obtained by a method-of-moments technique.

development of high-order/spectral methods on unstructured grids, the main results of the continued efforts in the analysis of PML methods, as well as the adaptation of the boundary variation methods to problems in diffractive optics. We shall conclude by discussing efforts related to finite-difference time-domain methods and techniques to improve on the widely used Yee scheme to enable correct treatment of interfaces and boundaries.

II.1 Structured Grid Multi-Domain High-Order/Spectral Methods

The straightforward application of spectral methods in several space dimensions requires that the computational domain is a square (in two dimensions) or a cube (in three dimensions) with the grid predefined by a tensorproduct of Gaussian points to assure the spectral accuracy.

In the structured grid multi-domain formulation these squares and cubes take the role of the fundamental building blocks by which the computational domain is filled to enable a high-order/spectral solution of Maxwells equations in a geometrically complex domain. Filling the computational domain is done in a completely body-conforming way, representing curvilinear material interfaces and metallic boundaries with an accuracy equal to that of the approximation. The computations in these elements involve the approximations of equations obtained by means of curvilinear transformations of Maxwells equations.

To connect the domains we exploit the hyperbolic nature of Maxwell equations along with the uniquely defined outward pointing normal vectors at the surfaces of the curvilinear elements to uniquely determine which information leaves and which enters the domain. Continuity of the characteristic variables is enforced strongly in a way entirely consistent with the physics of the problem. For interfaces placed between two materials we enforce the electromagnetic jump conditions to ensure correct behavior of the fields along such interfaces. This approach is likewise employed at geometric singularities such as vertices and edges combined with very weak filtering to ensure stability of the approximation.

Using these ideas, we have demonstrated the prospects of using high-order/spectral multi-domain methods for the accurate and efficient solution of nontrivial problems in electromagnetics

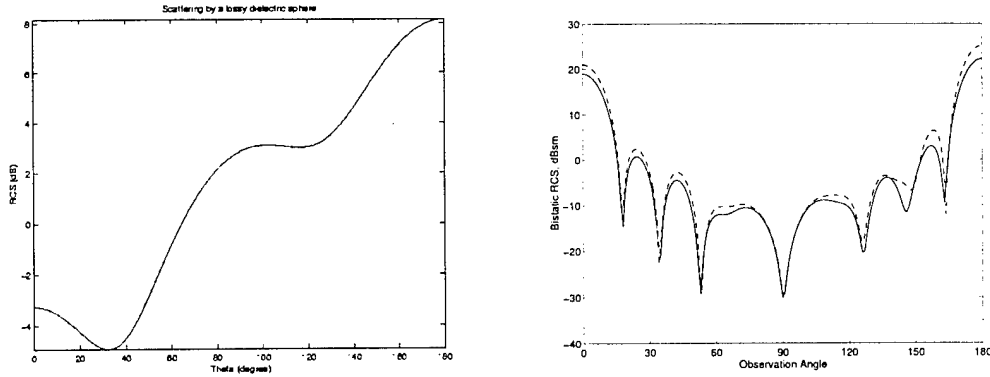


Figure 2: Numerical RCS result of scattering by a sphere (left) and a finite cylinder (right) of a 900MHz plane wave. Both bodies are composed of lossy di-electric materials with $\epsilon_r = 43.0$, $\mu_r = 1.0$, and $\sigma = 0.8\text{Sm}^{-1}$. The sphere has a radius of 0.1 meter, i.e., $ka = 0.6\pi$, and the length of the cylinder is 0.67m . The dashed line corresponds to the Mie-series result (left) and a finite element solution (right) respectively.

involving scattering by, and penetration into, geometrically complex two- and three-dimensional bodies.

As an example of current capabilities, consider the problem of scattering from an axisymmetric missile, assumed to be perfectly conducting. In Fig. 1 we illustrate a typical structured grid for the computation, emphasizing the fully body conforming grid and the geometric flexibility of the method. The validity of the results are confirmed by a direct comparison with a standard method-of-moments computations.

For the modeling of problems containing advanced materials, the development is currently ongoing and much additional work is needed. For problems with piecewise homogeneous materials, both two and three-dimensional tests have been successfully completed, confirming the accuracy and overall performance for scattering by spheres, cylinders, cubes etc.

As an example of the modeling of scattering by lossy materials we show in Fig. 2 the RCS computed using the three-dimensional framework for monochromatic scattering by a very dense sphere and a very dense cylinder with the latter being compared with results obtained using a very highly resolved finite element approach. The parameters of the materials are chosen to assemble those of human tissue.

Both the two and the three dimensional codes exploit the use of Perfectly Matched Layers (PML) to terminate the computational domains and specially designed PML methods for high-order methods have been implemented and thoroughly tested.

To enable the computational modeling of electrically large problems involving advanced materials, the potential for efficient implementations is critical. The existing codes have all been implemented using MPI to support fully parallel, distributed memory execution at a number of platforms, showing superior parallel performance

These results clearly establish that the recently developed two- and three-dimensional structured grid high-order/spectral multi-domain schemes are geometrically flexible, capable of handling real materials and allow for efficient implementations to enable the modeling of large and complex realistic configurations.

II.2 Unstructured Grid Multi-Domain High-Order/Spectral Methods

A concentrated effort has recently been initiated to develop methods for solving the time domain Maxwell's equations in complex geometries and media using an fully unstructured grid. The USEMe code (Unstructured Spectral Element Method) is the resulting implementation of a numerical scheme which employs nodal high-order/spectral multi-domain methods. Each component of the code has been carefully designed with efficiency, accuracy, flexibility, and robustness in mind.

The standard geometric building block by which the computational domain is gridded in USEMe is the triangular element in 2D, and the tetrahedral element in 3D. This allows for the use of standard finite element or finite volume type meshes using these elements to describe arbitrarily complex domains, hence overcoming one of the main concerns associated with the structured grid methods. The use of triangles and tetrahedrons remains one of the most important design principles of the method as it enables a tight integration with industry standard mesh generators.

USEMe is based on penalty/discontinuous Galerkin (DGM) type scheme, which is a particular form of a penalty scheme that guarantees elemental conservation and global stability. Neighboring elements are patched together through the use of penalty terms to account for jumps across their shared boundary. This formulation has the advantage that it allows material coefficients to vary discontinuously at the interface between two elements, while still preserving high order accuracy. Additionally this allows for efficient communication in parallel computations.

A thorough convergence analysis for the proposed framework has been completed, putting the expectations on firm ground and verifying that one can indeed expect the properties speculated during the initial developments and essential as a motivation for the chosen approach. The analysis also includes bounds on the divergence error, confirming that the computed results remain divergence free to the order of the scheme away from singular points.

A general two-dimensional unstructured grid code, based on the use of curvilinear triangles, has been implemented and tested extensively, including by third party users. The code is flexible, versatile, and robust, allowing for the modeling a very general two-dimensional (TE and TM) time-domain scattering, penetration and radiation problems involving di-electric and magnetic materials, possibly of a lossy nature.

The discretization provides a fully body-conforming high order representation of a material scatterer, hence overcoming the staircasing phenomena evident in common finite difference schemes. In Figure 3 we illustrate some elements which have an edge on the boundary. Their nodes have been mapped to the boundary and the internal nodes blended linearly from the boundary. The full triangulated region is likewise illustrated.

As an example of the expected accuracy, we compute plane wave scattering from a PEC cylinder with the non-uniform near-field mesh illustrated in Fig. 3. This is an excellent test case as it allows us to determine the performance of the PEC boundary conditions, PML boundary truncation, RCS calculation, curvilinear body representation and high order approximation techniques. Comparing the computed z component of the electric field with the exact solution over the interior domain, Table 1 confirms exponential convergence. Numerous other results for scattering and penetration into simple homogeneous scatterers have shown similar accuracy. Other more complex problems involving materials and singular solution behavior display a very similar accuracy and overall performance.

Serial as well as fully parallel implementations have been completed and various tools such

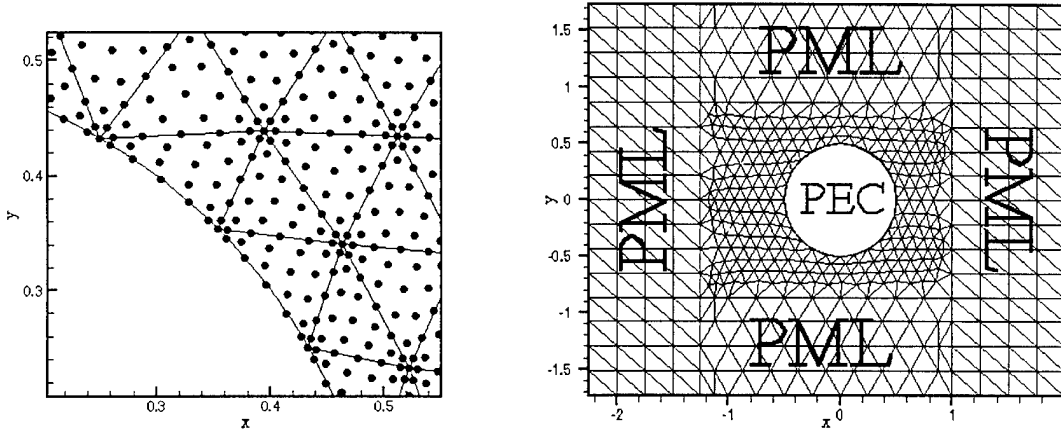


Figure 3: Left: Seventh order boundary fitted triangular elements. Right: Full triangulated region for two-dimensional scattering with PML.

Expansion	L_∞ error
8	3.2E-02
10	2.1E-03
12	6.2E-04

Table 1: L_∞ error over the interior domain as function of expansion order for scattering of a TM plane wave from a PEC cylinder ($ka = 7\pi$).

as near-to-far-field transformations and highly efficient absorbing layer techniques have been implemented and tested. The code has been interfaced with a public domain grid-generator to enable simple and user-friendly grid-generation.

The development of a general three-dimensional framework is, by the sheer complexity of the problem, a daunting task and it remains a work in progress. A general, three-dimensional version of the scheme has been implemented and initial tests have been conducted, verifying the expected accuracy and overall performance. So far, these test cases have been limited to problems involving purely metallic scatters, although this remains less of a concern as pure metallic scattering often provides the most challenging test cases.

As a simple test of the current capability of the framework we show in Fig. 4 the bistatic RCS for a $ka = 10$ PEC sphere as computed using the unstructured framework and compared with the analytic Mie-series. As expected we find excellent agreement.

As a more eye-catching, and preliminary, result Figure 5 demonstrates that the code is currently capable of simulating electromagnetic plane wave scattering from a complex F15 type geometry. Even though this is a preliminary result, the code is capable of representing much more complex media and also more complex and higher frequency signals than this monochromatic example. This result was obtained by running on a single processor workstation using third order accurate elements. Higher resolution calculations are being performed in parallel on an IBM SP.

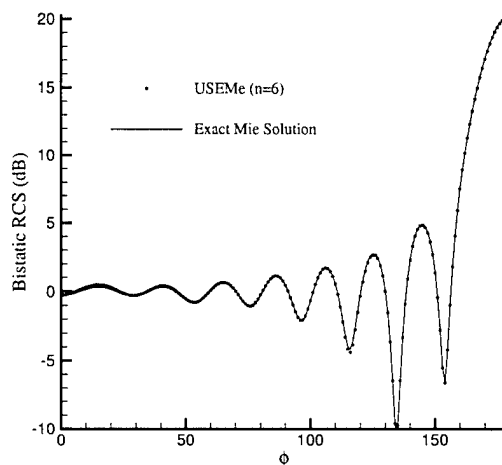


Figure 4: Bistatic RCS for $ka = 10$ as computed using the unstructured grid framework with an 6'th order basis.

A fully parallel version, implemented in MPI and Fortran/C, has been tested, showing excellent parallel speed up which remains a crucial property to enable the modeling of large scale problems of realistic complexity. The parallel performance is illustrated in Table 2, confirming that the code attains up to 95 percent parallel efficiency as the number of processors is increased.

Expansion Order	Total Degrees of Freedom	# of processors			
		2	4	8	16
3	7,380,000	5.6	3.4	1.8	.95
4	14,760,000	**	7.4	3.9	2.3
5	25,830,000	**	**	7.8	4.3

Table 2: Wall clock time per Runge Kutta integration stage. Timings taken on an IBM SP2 at CASCV, Brown University. (** implies that there was not enough memory local to the nodes)

The code has been interfaced with Gambit/Fluent grid-generator to allow for a user-friendly approach to the daunting of three-dimensional grid-generation. This interfacing has been accomplished through a pre-processing module that enables the use of a standard finite-element/finite-volume grid in a fully body-conforming high-order accuracy framework. It is worth emphasizing that there is nothing special about the chosen grid-generator and any finite-element/finite-volume grid generator can be used as a frontend to USEMe, provided only that a simply format-interface be implemented.

II.3 Absorbing Boundary Conditions for Time-Domain CEM

One of the central issues in time domain CEM is the development of techniques for the truncation of the infinite computational domain in such a way that outgoing waves leave the domain without reflections which could otherwise reenter and eventually falsify the computational results.

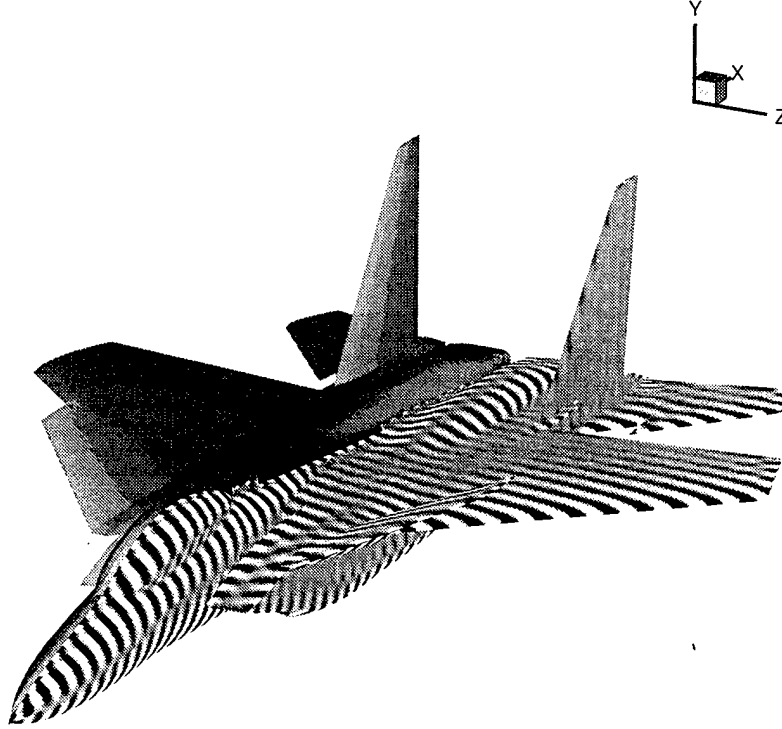


Figure 5: Nose to tail component of the reflected magnetic field from an incident plane wave.

In 1994 Berenger introduced a new methodology for designing such schemes by the introduction of an absorbing layer, to which he attributed material properties that modify the vacuum-equations so that the field strength decays. In his original paper these material properties were based on a mathematical construct, involving splitting the transverse magnetic field.

We have previously conducted a detailed mathematical analysis of the PML formulation applied to the two dimensional transverse-electric mode (TE) of Maxwell's equations. The conclusions of this analysis hold also for all other forms of the equations. We were interested in the well-posedness of the PML formulation, and therefore investigated the pure-initial value problem. The main conclusion is that the PML split-form of Maxwell's equations is only weakly well-posed and therefore its solution could diverge under small perturbations. This theoretical result has some far reaching conclusions. First, it indicates the the split field PML will have problems as the required number of points in the PML layer will increase with time. Moreover, since all physical system describing reality must be strongly well posed, the PML can not represent any physical layer.

In the case of the transverse electric (TE) case or transverse magnetic (TM) these considerations lead to a set of 4 p.d.e.'s, different from those given by Berenger.

The dimensionless form of the equations based on the Lorentz-material model, is:

$$\frac{\partial E_x}{\partial t} = \frac{\partial H}{\partial y} - J, \quad \frac{\partial E_y}{\partial t} = -\frac{\partial H}{\partial x} - \sigma E_y$$

$$\frac{\partial H}{\partial t} = \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} - \sigma H, \quad \frac{\partial J}{\partial t} = -\sigma \frac{\partial H}{\partial y}$$

where J is a polarization current.

We showed that the set of 4 p.d.e.'s can be reduced to a set of 3 inhomogeneous Maxwell equations augmented by a temporal O.D.E. This means that the original set of equations in the layer is strongly well posed. We then provide a closed form solution for plane -waves traveling in the absorbing layer, under the assumption of periodicity in y , for 2 cases – the semi-infinite layer and the finite layer. The analysis confirmed that the infinite layer is a true PML but also exposed that the finite width Lorentz material PML may exhibit locally growing solutions before they finally decay.

The method of deriving absorbing layers from physical considerations has limitations. In particular the absorbing properties of the layers can not be controlled. We have developed a mathematical methodology for the construction of PMLs. This methodology is more flexible than the physically motivated one and it allows control of the decay properties of the solution in the absorbing layer. One of the possible sets is given by

$$\begin{aligned} \frac{\partial E_x}{\partial t} &= \frac{\partial H}{\partial y} \\ \frac{\partial E_y}{\partial t} &= -\frac{\partial H}{\partial x} - 2\sigma E_y - \sigma P \\ \frac{\partial H}{\partial t} &= \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} + \sigma' Q \\ \frac{\partial P}{\partial t} &= \sigma E_y, \quad \frac{\partial Q}{\partial t} = -\sigma Q - E_y \end{aligned}$$

The solution vector now is given by

$$\begin{pmatrix} E_x \\ E_y \\ H \\ P \end{pmatrix} = \begin{pmatrix} -\beta \\ \alpha \left(\frac{i\omega}{\sigma + i\omega} \right) \\ 1 \\ \frac{i\beta\sigma^2}{\omega} \end{pmatrix} e^{i\omega(t - \alpha x - \beta y)} e^{-\alpha \int_0^x \sigma(\eta) d\eta}$$

The solution here is bounded by a function that does not grow in any direction

The success of the PML method is crucial in applying high order accuracy methods to the simulations of Maxwell equations. After all, there is no point in achieving high accuracy in the computational domain if the reflections introduce large errors. The PML methodology minimize the numerical reflections.

However it was found that all the known PML allow linear (and non-physical) growth in time when simulating pulses. It seems that the growth is triggered when the pulse leaves the domain and the solution vector approach constant in space. A simple analysis explains the situation. Consider the physically based PML, and assume that the spatial derivative vanish, then the equations for E_x and J decouple and they display a linear growth in time. It is easy, based on this analysis, to find a "cure" for this problem. However it is not clear if the corrected method is still a PML. This problem remains open. The numerical experiments indicate that the corrected, physically motivated, PML maintains its absorption properties even with the time stabilizing term. A better analysis and more experiments are needed to have the full understanding of this very important question.

II.4 Boundary Variation Techniques for Waveguide Holograms

It has recently been established by Bruno and Reitich that solutions to electromagnetic diffraction by a periodic structure depend analytically on the variations of the interface. In other words, diffraction from a periodic grating can be determined from knowledge of reflection and refraction at a plane interface and the diffraction problem be solved by analytic continuation. Using this result, a high-order perturbation technique was developed for finite-size perturbations and successfully used it in modeling diffraction by two and three-dimensional metallic and transmission gratings.

To utilize and further generalize on these results we have initiated work on the formulation and implementation of boundary variation techniques for the analysis and modeling of waveguide grating couplers. These are diffractive optical devices in which a guided wave in a thin-film waveguide is coupled to free-space radiation through a surface relief. These problems are vastly different from what was previously considered. Among other things, the illuminating wave is a guided wave with evanescent tails. Furthermore the diffraction process includes multiple refraction/reflection processes. Finally, we have extended the analysis to structures of finite extent.

M	P ($\cdot 10^{-2}$)
2	1.208589
4	1.220834
6	1.220247
8	1.220243
10	1.220243

Table 3: Power in the -1st diffraction order for different number of terms $[M,M]$ in the Padé approximation to the power series expansion.

As a first example of the performance of the boundary variation scheme, consider a waveguide structure consisting of a core layer with refractive index $n = 1.45$ and thickness $d_1 = 0.8$, sandwiched between two cladding layers of refractive index $n = 1.4$. The top cladding layer has a finite thickness of $d_2 = 1$ and above this layer is air with $n = 1$. For the fundamental TE mode this geometry yields an effective index of 1.4213.

We consider a cosine surface relief

$$f_\delta(z) = A \cos\left(\frac{2\pi}{\Lambda}z\right) \quad (1)$$

Let us first study the convergence of the scheme. As we do not have an analytic solution to compare with, we are unable to compute the error. Rather, we look at the power coupled to the -1st diffraction order as we increase the number of terms in the Padé approximation to the Taylor series expansion of the global solution. Table 3 confirms the convergence in the case of $A = 0.1$ as the number of terms in the power series expansion increases.

Let us now demonstrate the use of the proposed boundary variation method to study aperiodic surface-relief gratings couplers of finite length. Clearly, as we use a periodic Rayleigh series expansion for the radiated fields, the grating is implicitly forced to be periodic. However, as we shall demonstrate, choosing a sufficiently large total length of the computational domain as

compared with the length of the finite surface relief, the results becomes consistent with those obtained using a method dealing with truly finite gratings.

For the FGC surface relief we use the generic profile

$$f_{\delta}(z) = A \exp \left[- \left(\frac{z - z_0}{w} \right)^2 \right] \cos [2\pi (a_0 + a_1 (z - z_0)) (z - z_0)] \quad (2)$$

where A is the amplitude, w is the width of the exponentially truncated relief, z_0 is the center of the relief, $a_0 = 1/\Lambda$ for the unchirped relief, and a_1 is the chirp parameter. We consider, as an example, the parameters $A = 0.25$, $a_0 = 1.4213$, $a_1 = 0.005$, and $w = 3$ and show in Fig. 6 that there is an excellent agreement between the farfield patterns of the results obtained even for this relatively deep surface relief grating and those computed with a rigorous spectral multi-domain scheme solving Maxwells equations directions and to very high order.

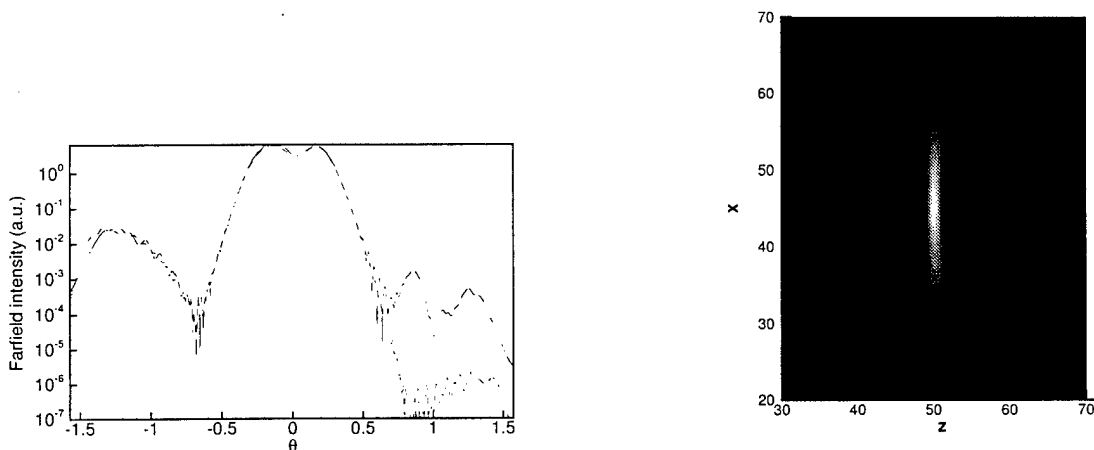


Figure 6: Left: Farfield radiation patterns for FGC computed using the boundary variation method (dashed) and a spectral multi-domain method (solid). Right: Focusing beam emanating from grating coupler at $x=0$.

A	M		f	time	
	BV	BV		SC	BV
0.1	7	47.1	47.0	46s	30h
0.2	13	46.3	46.2	390s	64h
0.3	17	45.2	45.1	1081s	126h

Table 4: Key figures for spectral collocation (SC) and the proposed boundary variation (BV) computations. A is the amplitude of the surface relief. An $[M,M]$ Padé approximant is used for the BV method. f is the focal length normalized with the free-space wavelength, and time reflects the total computation time.

We find excellent correspondence in the farfield maintained in the nearfield even though the intensity is slightly lower for the BV method for all amplitudes, which may be due to not accounting for multiple reflections. Looking at the computation time in Table 4, it is evident that the use of the approximate boundary variation method certainly pays off: While we find excellent agreement with the rigorous spectral collocation method, we find a reduction in the computation time exceeding a factor of 2000 is achievable, a fact which calls for the future use of the method as the forward solver in an optimization scheme.

II.5 Embedded Interface Finite-Difference Methods

While it is well known 4th order methods perform significantly better than 2nd order methods when solving wave problems, it is also well known that stable 4th order finite difference schemes can be constructed on equidistant Cartesian grids even as one approaches the boundary and one-sided closures are required. A central difficulty, however, is introduced in the need to treat geometrically complex objects. Rather than adapting a multi-element formulation we wish to overcome this complication while maintaining a very simple Cartesian grid and embed the whole computational problem into the grid. The success of such embedding techniques hinges critically on the formulation of the finite difference stencils in a way that allows for the including the position of the embedded objects as well as the boundary conditions of the field on the surface of the objects.

Attempts to construct stable and well behaved finite difference schemes that allows one to use a simple Cartesian grid for solving partial differential equation in geometrically complex settings is not new. In particular for solving the incompressible Navier-Stokes equations can one find a wealth of methods which all seem to have their origin in the immersed boundary method. For problems involving transparent boundaries, as is generally the case for problems in electromagnetics, it is necessary to seek an approach in which one directly imposes the correct interface conditions on the solution across the interface. An approach used extensively in the context of electromagnetics is to simply assign averaged material properties to grid points at the material interface, although we have shown this approach yields 1st order accuracy at best.

In very recent work, we have proposed a novel 2nd order finite difference based approach for solving Maxwells equations but directly applicable to wave problems in general. Contrary to previously proposed methods, it is equally applicable to the scalar and the system case, the bulk of the work involved in treating the material interfaces is performed in a preprocessing phase, and the scheme handles generally curved internal interfaces as well as fully reflecting boundaries with equal ease and in a uniform way.

Although the thorough theoretical developments are completed for the one-dimensional problem only, the approach generalizes to several dimensions without complications. Consider, as an example, the electromagnetic scattering of a plane wave impinging on a two-dimensional di-electric cylinder. In Fig. 7 is shown the temporal behavior of the global error as well as a resolution study at a specific time. We see, as expected, that incorrect staircased treatment of boundaries and their position severely limits the accuracy of the simple Yee scheme. Contrary to this, the new scheme is truly second order and typically yields at least an order of magnitude improvement in accuracy over the Yee scheme for the same resolution and, thus, the same computational work. In other words, one can improve the accuracy at little or no cost or one can obtain results of a comparable accurate accuracy at dramatically reduced computational cost.

Current efforts include the continued verification of the two-dimensional framework for both polarizations as well as the initial phase of the implementation and testing of a general three-dimensional framework.

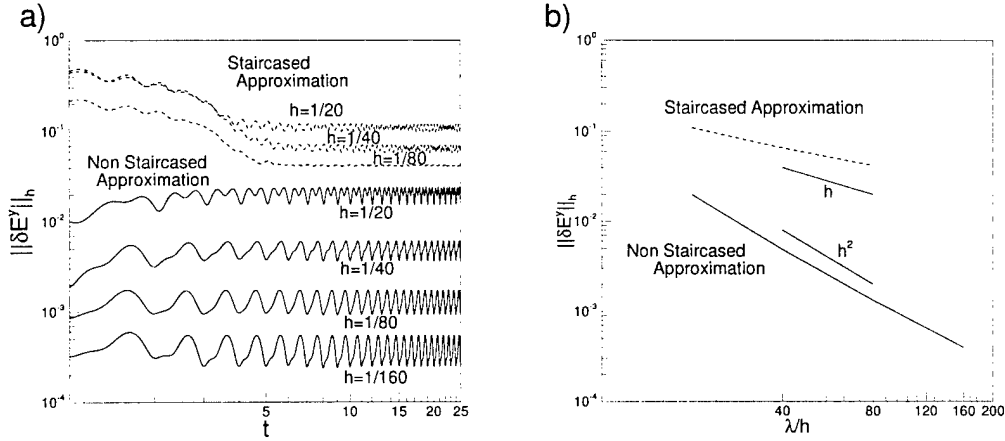


Figure 7: In a) we show the temporal dependence of the global L^2 error of E for different resolution in terms of the free-space wavelength for the staircased and non staircased approximation. In b) is shown the global error at $t=25$, illustrating the expected convergence rate.

III. Papers Citing Support from Grant

III.1 Appeared or Accepted

- A. Ditkowski, K. H. Dridi, and J. S. Hesthaven, 1999, *Convergent Cartesian Grid Methods for Maxwells Equations in Complex Geometries*, J. Comput. Phys. - to appear.
- K. H. Dridi, J. S. Hesthaven, and A. Ditkowski, 1999, *Staircase Free Finite-Difference Time-Domain Formulation for General Materials in Complex Geometries*, IEEE Trans. Antennas Propaga. - to appear.
- D. Gottlieb and J. S. Hesthaven, 2000, *Spectral Methods for Hyperbolic Problems*, J. Comput. Appl. Math. - to appear.
- T. Warburton, L. Pavarino and J.S. Hesthaven, 2000 *A Pseudo-Spectral Scheme for the Incompressible Navier-Stokes Equations Using Nodal Elements*, J. Comput. Phys. **163**(2000), pp. 1-21.
- V. Zharnitsky, E. Grenier, S. K. Turitsyn, C. K. R. T. Jones, and J. S. Hesthaven, 2000, *Ground States of Dispersion Managed NLS*, Phys. Rev. E. **62**(5), pp. 7358-7364.
- J. S. Hesthaven and C. H. Teng, 2000, *Stable Spectral Methods on Tetrahedral Elements*, SIAM J. Sci. Comput. **21**(6), pp. 2352-2380.
- P. G. Dinesen and J. S. Hesthaven, 2000, *A Fast and Accurate Boundary Variation Method for Diffractive Gratings*, J. Opt. Soc. Am. A **17**(9), pp. 1565-1572.
- J. S. Hesthaven, 2000, *Spectral Penalty Methods*, Appl. Numer. Math. **33**(1-4), pp. 23-41.
- B. Yang and J. S. Hesthaven, 2000, *Multidomain Pseudospectral Computation of Maxwell's Equations in 3-D General Curvilinear Coordinates*, Appl. Numer. Math. **33**(1-4), pp. 281-289.

- P. G. Dinesen, J. S. Hesthaven and J. P. Lynov, 2000, *A Pseudospectral Collocation Time-Domain Method for Diffractive Optics*, Appl. Numer. Math. **33**(1-4), pp. 199-206.
- J. S. Hesthaven, P. G. Dinesen and J. P. Lynov, 1999, *Spectral Collocation Time-Domain Modeling of Diffractive Optical Elements*, J. Comput. Phys. **155**(1), pp. 287-306.
- S. Abarbanel, D. Gottlieb and J. S. Hesthaven, 1999, *Wellposed Perfectly Matched Layers for Advective Acoustics*, J. Comput. Phys. **154**(2), pp. 266-283.
- P. G. Dinesen, J. S. Hesthaven, J. P. Lynov and L. Lading, 1999, *Pseudospectral Method for the Analysis of Diffractive Optical Elements*, J. Opt. Soc. Am. A **16**(5), pp. 1124-1130.
- B. Yang and J. S. Hesthaven, 1999, *A Pseudospectral Method for Time-Domain Computation of Electromagnetic Scattering by Bodies of Revolution*, IEEE Trans. Antennas Propaga. **47**(1), pp. 132-141.
- P. G. Dinesen and J. S. Hesthaven, 2000, *Analysis of Grating Couplers Using the Boundary Variation Method*. In Technical digest. Diffractive optics and micro-optics meeting and table top exhibit, Quebec City (CA). Optical Society of America, OSA Technical Digest series, pp. 84-86.
- P. G. Dinesen and J. S. Hesthaven, 2000, *Rigorous 3-D Analysis of Focusing Grating Couplers Using a Spectral Collocation Method*. In Technical digest. Diffractive optics and micro-optics meeting and table top exhibit, Quebec City (CA). Optical Society of America, OSA Technical Digest series, pp. 81-83.
- P. G. Dinesen, J. S. Hesthaven, and J. P. Lynov, 2000, *Rigorous Analysis of Focusing Grating Couplers Using a Time-Domain Spectral Collocation Method*. In Diffractive/holographic technologies and spatial light modulators 7. Optoelectronics 2000, San Jose, CA. Cindrich, I.; Lee, S.H.; Sutherland, R.L. (eds.), (International Society for Optical Engineering, Bellingham, WA, 2000), Proceedings of SPIE **3951**, pp. 11-19.
- P. G. Dinesen, J. S. Hesthaven, and J. P. Lynov, 2000, *Rigorous Three-Dimensional Analysis of Surface-Relief Gratings Using a Spectral Collocation Method*. In Diffractive/holographic technologies and spatial light modulators 7. Optoelectronics 2000, San Jose, CA. Cindrich, I.; Lee, S.H.; Sutherland, R.L. (eds.), (International Society for Optical Engineering, Bellingham, WA, 2000), Proceedings of SPIE **3951**, pp. 2-10.
- K. Dridi and J.S. Hesthaven, 1999, *N-space Staircase-Free Finite-Difference Time-Domain Formulation for Arbitrary Material Distributions: Numerical Investigations on a Focusing Grating Coupler in Dielectric Waveguides*. Proc. of Integrated Photonics Research IPR 99, Santa Barbara, CA. pp. 250-252.
- P. G. Dinesen, L. Lading, J. P. Lynov and J. S. Hesthaven, 1998, *Waveguides and Diffractive Elements for Non-Contact Sensors: Analysis* Proc. of Diffractive Optics and Micro-Optics, Hawaii. pp. 209-211.
- J. S. Hesthaven, P. G. Dinesen and J. P. Lynov, 1998, *Pseudospectral Time-Domain Modeling of Diffractive Optical Elements*. Proc. of The 14'th Annual Review of Progress in Applied Computational Electromagnetics, Monterey, CA. pp. 858-865.

- B. Yang, D. Gottlieb and J. S. Hesthaven, 1997, *On the Use of PML ABC's in Spectral Time-Domain Simulations of Electromagnetic Scattering*. Proc. of The 13'th Annual Review of Progress in Applied Computational Electromagnetics, Monterey, CA. pp. 926-933.
- D. Gottlieb and P. Fischer, *On the optimal number of subdomains for hyperbolic problems on parallel computers*, Int. J. of Supercomp. Appl. and High Perf. Comp. 11(1997), pp. 65-76.
- D. Gottlieb and S. Abarbanel, *A Mathematical Analysis of PML Methods*. J. Comput. Phys. 134(1997), pp.357-363.
- M. Carpenter, J. Norstrom, and D. Gottlieb, *A Stable and Conservative Interface Treatment of Arbitrary Spatial Accuracy*, J. Comput. Phys. 148(1999), pp.341-365.
- S. Abarbanel, D. Gottlieb and E. Turkel, *Analysis of the Error for Approximations to Systems of Hyperbolic Equations*, J. Comput. Phys. 151(1999), pp. 997-1007.

III.2 Submitted

- P. G. Dinesen and J. S. Hesthaven, 2001, *A Fast and Accurate Boundary Variation Method for Diffractive Gratings II. The Three-Dimensional Vectorial Case*, J. Opt. Soc. Am. A - submitted.
- J. S. Hesthaven and T. Warburton, 2001, *High-Order/Spectral Methods on Unstructured Grids. I. Time-Domain Solution of Maxwell's Equations*, J. Comput. Phys. - submitted.
- C. H. Teng, A. Ditkowski, and J. S. Hesthaven, 2000, *Modeling Dielectric Interfaces in the FDTD-Method: A Comparative Study*, IEEE. Trans. Antennas Propaga. - submitted.
- P. Dutta, T.C. Warburton, and A. Beskok, 2000, *Analysis of Electroosmotically Driven Micro-Channel Flows*, J. of Fluid Mech. - submitted.
- A. Beskok and T.C. Warburton, 2000, *An Unstructured H/P Finite Element Scheme for Fluid Flow and Heat Transfer in Moving Domains*, J. Comput. Phys. - submitted.

III.3 Theses Completed

- C. H. Teng, *Numerical Methods for Wave Problems in Complex Geometries*, PhD thesis. Division of Applied Mathematics, Brown University, 1998-2001.
- B. Yang, *Spectral Methods and Absorbing Boundary Conditions for Maxwell's Equations*, PhD thesis. Division of Applied Mathematics, Brown University, 1995-1998.